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Some observations regarding the detonation of nitromethane

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The purpose of this document is to summarize the pertinent detonation-related properties of nitromethane (NM) from an expansive body of literature.

Industrial NM (>98-99% purity) is an insensitive homogeneous liquid secondary explosive. Sustained input shock pressure of > 7 GPa are required to produce relatively prompt shock-to-detonation (SDT) proceeding at Chapman-Jouguet (CJ) conditions [1, 2]. Owing to the low density and relatively compressible nature of liquids such as NM, it has a low shock impedance compared with most metallic materials, and so it is extremely difficult for realistic accident scenarios to generate these high pressure shock conditions where prompt CJ SDT occurs. In fact, provided that the liquid is packed into steel drums of less than 55 US gallons, road and rail transport rules allow the liquid to be handled and stored as a flammable solvent rather than an explosive [3].

Owing to the transparent nature of NM and the fact that the homogeneous detonation phenomenon in NM can be changed to a heterogeneous response by the addition of sparse solid particles, NM has been the subject of much study [4, 5, 6, 7]. Additionally, the initially insensitive nature of NM can be

made much more sensitive by the addition of a low weight percentage of a number of base liquids such as DETA [8, 9, 10]. The result is a fairly ideal, cap sensitive, powerful explosive with low critical diameter, but with a limited shelf-life.

Chemistry

Although the structure of NM is relatively simple, there is some debate regarding the exact decomposition pathways under anaerobic conditions (e.g. detonations that are principally designed to push metal). The simplest path is as follows,

$$2\,CH_3NO_2 \longrightarrow 2\,CO + 2\,H_2O + H_2 + N_2$$

However, the Cheetah code predicts a more complex breakdown with trace amounts of other products, principally NOx, and estimates an anaerobic energy output of detonation of 4.622 kJ g^{-1} [11]. What is not in doubt is that the reactions leave considerable free hydrogen and carbon monoxide in the products. Detonations performed in ambient air will therefore exhibit significant post-detonation mixing and re-combustion of the hot products when mixed with oxygen. This results in greater heating of the products at late time. Assuming perfect mixing in copious air, Cheetah predicts an energy release of 10.56 kJ g^{-1}, a factor of approximately 2 higher than under anaerobic situation. This additional energy leads to enhanced blast effects at intermediate and far-field locations. Such enhancement will not occur under anaerobic conditions such as detonation in an inert or low pressure atmosphere, or where large charges are detonated in tunnels or boreholes where the charge fills the majority of the available volume.

Velocity of Detonation & Critical Diameter

There are many papers listing the velocity of detonation in NM. Inferring the steady-state velocity of detonation (VOD) at infinite diameter is difficult, being both a function of chemical purity, temperature and technique. Studies in long brass tubes produce a value of ≈ 6.25 mm μs^{-1} [12]; however, most researchers use a figure of $\approx 6.3 - 6.35$ mm μs^{-1} for practical charge sizes [4]. The density of NM (1.137 g/cc at 20°C) is a relatively strong function of temperature in comparison with many explosives. The density in g/cc as a function of temperature in Celsius is [4],

$$\rho = 1.1615 - 1.1952 \times 10^{-3} t - 1.553 \times 10^{-6} t^2. \quad (1)$$

Density, together with a small effect on the energy barrier to reaction from the starting temperature, results in VOD being a moderate function of temperature. Campbell measured -3.7 m s^{-1} K^{-1} over a temperature range -20 to 62°C with a VOD of ≈ 6.25 mm μs^{-1} at 22°C [13, 14].

Being a measure of the ideality of a detonation, the critical diameter and shock front curvature of NM has been extensively studied. However, the confinement used has a great influence on the values measured. The majority of researchers have standardized on circular Pyrex tubes of varying wall thicknesses to confine the liquid, since they used optical access to make other measurements. Pyrex is a reasonable impedance match to detonating NM. Asay measured a critical diameter of 16.4 ± 1.1 mm [8] and Campbell [14] studied the effect of temperature on failure diameter noting a reduction of approximately 50% for a 40K increase in initial temperature.

Confinement in metal (a high impedance material) has a dramatic effect on lowering the critical diameter. Using brass tubes, a critical diameter of only $\approx$2.2 mm was found at room temperature [12]. Experiments using aluminum confinement have been performed looking at the ratio of tube diameter to slab separation thickness, and a critical diameter of 2.5 mm was measured [15]. For standard explosives, a critical slab separation thickness of 50% of the

critical diameter is observed. In NM, a different ratio of 30% was established, suggesting more complex behavior perhaps relating to the cellular detonation phenomenon described later. However, it should be noted that the longitudinal sound speed in aluminum (≈ 6.3 mm μs^{-1}) is very close to the detonation velocity of NM, suggesting that the aluminum confinement could have influenced the results of both the slab and tube measurements owing to enhanced support of the detonation from the boundary condition.

The effects of deuterating NM have been studied and reveal that the VOD decreases and the failure diameter increases. Typically, an increase in explosive density is expected to increase VOD; however, in this case the extra parasitic mass of the deuterium reduces the available detonation energy per mole, thus explaining the decreased performance [12]. The extra neutron mass also slows the rate of detonation-supporting reactions and results in a less ideal explosive with a correspondingly greater failure diameter.

Detonation shock front curvature is known to reduce the local velocity of detonation owing to divergent flow energy losses. One way that this behavior is captured is by a scheme known as Detonation Shock Dynamics (DSD) that lends itself to a fast-running computer algorithm for explosive modeling by modifying a programmed burn set for local curvature effects. DSD is currently only valid for convex curvature (VOD locally slowed), not concave curvature where an overdriven detonation is created (VOD locally increased). Some DSD parameters for NM have been published [16].

Reaction Zone

Understanding any measurements made in the reaction zone of detonating NM rely on an understanding of the physical parameters of the explosive in question for interpretation. It is difficult to measure the unreacted equation of state (EOS) of explosives at pressures close to the CJ point owing to the onset of reaction disturbing the intended measurement. NM is no exception and so typically the unreacted EOS is an extrapolation of measurements made at

lower pressures. The simplest approach is a Mie-Gruneisen EOS mixed with a fixed Gruneisen gamma value and specific heat at constant volume (C_V). One accepted set of parameters in SI units is,

$$U_s = 1647 + 1.637U_p, \tag{2}$$

where U_s is the shock velocity and U_p the particle velocity [17]. Another is,

$$U_s = 1760 + 1.56U_p, \tag{3}$$

with an assumed initial density of 1.128 g/cc [18]. Estimates of the Gruneisen gamma appear to have been calculated, but not measured, and vary between 0.7 and 1.4 over the pressure range of interest for detonation studies [19, 20, 21]. As stated earlier, pure NM exhibits homogeneous detonation phenomena and this is most commonly modeled by an Arrhenius kinetics approach towards decomposition. That is, the reaction is driven by bulk NM temperature, not via local hot-spots generated by a shock passing through regions with imperfections, as with most solid phase explosives [7]. As such, accurate estimates of temperature in shocked liquid are vital if accurate behaviors are to be captured. It has been calculated that the C_V of NM varies from approximately 1250 J kg^{-1} K^{-1} at room temperature to approximately 1900 J kg^{-1} K^{-1} close to decomposition temperatures [19]. Therefore, models based on fixed parameters are likely to prove unreliable in practice. Semi-analytical models of the unreacted EOS for NM relying on variable physical parameters have been created and have been compared with experimental data on temperature rise, but they would be costly to compute in real time within a wider modeling context [20, 21].

An alternative and probably more accurate method is to generate tabular EOS values for both unreacted and reacted NM populated with pressures, volumes, temperature and internal energy over a wide range of practically significant values [7]. Such tables are unconstrained by the need for constant parameter values, single material phases and similar analytical simplifications, and can be fitted via the use of data from multiple sources. What is then

required to model the detonation is a set of reaction rate equations that transform the unreacted EOS into the reacted one with suitable physical constraints (pressure and temperature conditions between the materials etc.). As stated previously, reaction rates based on Arrhenius kinetics are likely to be the most fruitful for materials such as NM.

Owing to the exceptional temporal resolution required to make reaction zone measurements in explosives, typically optical velocimetry techniques are employed to measure the particle velocity at an interface between a reacting explosive and a stress-maintaining transparent material interface (a 'window'). Various researchers have attempted to make such measurements on NM including resolving the Von-Neumann spike (VN), the CJ point (the sonic locus) and the pressure in the following flow [18, 22]. Diagnostics embedded in the detonation explosive would be superior if a technique with high temporal resolution could be created. Currently, such embedded techniques have a temporal resolution of $\approx$50 ns making them all but useless for studies of the reaction zone. The difficulty with using a window is that the detonation is disturbed. It is not possible for the window to simultaneously match the impedance of the unreacted explosive and the reacted state. That is, a shock, or a release, is sent backwards into the reaction zone from the window interface depending on the explosive properties and those of the window. Thus, the very process being interrogated is disturbed at the same time that a supported shock in the explosive becomes an unsupported one in the window. Nevertheless, such optical techniques are the best that can be achieved at this current time.

Unfortunately, it has proven difficult to measure the extremely transitory VN spike accurately and after a rapid drop in pressure, the region where the CJ pressure is expected to be located is in a fairly flat region of the particle velocity path and no abrupt distinguishing change in slope occurs. The break in gradient of the U_p versus time plot indicates that both a fast and slow reaction rate is operating. Because the speed-of-sound in the gas is a function of the derivative of the isentrope, establishing the sonic locus this way is prone to error. Recall that energy released from later time reactions behind the

sonic plane cannot support the detonation since the additional energy cannot reach the primary shock front. Thus, estimates of the VN and CJ points are reliant on extrapolations from the unreacted EOS measurements, theoretical chemistry generated reacted EOS curves and other physical measurements such as velocity of detonation and initial density.

Nevertheless, the attempts at measuring the reaction zone are not in disagreement with theoretical models, but are not currently precise enough to constrain the fitting parameters more tightly. Studies of pure NM and NM sensitized with DETA show that the initial reaction rate is accelerated, but not the later reactions within the sonic region [18]. This initial reaction is estimated to last 5–10 ns and this corresponds to the very short estimate of reaction zone length inferred by Engelke from shock front curvature analysis [10]. Using a 2 ns resolution VISAR system, it has proven difficult to accurately resolve the VN spike [22]. It is estimated that the sonic plane lies 100-150 ns behind, corresponding to a reaction zone length of 600-900 μm. This assumes a CJ pressure of $\approx$12.5 GPa. That figure is consistent with many other researchers' assumptions [4], but is in disagreement with Menikoff & Shaw [7] who argue, after reviewing a large body of research and modeling, that the CJ pressure is actually significantly lower at $\approx$10.5 GPa. A lower value would correspond to a longer reaction zone length and suggest a less ideal explosive performance. Using an optical technique with approximately a 1 ns temporal resolution, it is thought that the VN spike was still not quite resolved because a peak velocity of 2.5 rather than 2.6 mm μs^{-1} was measured at the window interface. A value of 2.6 mm μs^{-1} corresponds to the expected VN pressure of 20 GPa [18].

Corner Turning

There appears to have been relatively little study of corner turning in NM. Only two experimental papers have been identified: the first is hard to obtain [6] and the second is mostly in Chinese [23]. Therefore, this section will have

more detail and analysis than others in this document to explain the effect and describe some new modeling efforts.

Corner turning describes what happens when there is an abrupt change in cross-section of a detonating explosive from smaller to larger; see figure 1. As the detonation breaks out from the smaller cross-section, the wave must diffract as a divergent process into the larger cross-section. The finite reaction zone in any real explosive will affect the planarity of the detonation in the smaller cross-section; however, at the transition in areas, both side-releases between the lead shock and the sonic plane distance will erode the detonation and the convex curvature will require greater energy to support detonation than required for pseudo-1D detonation. These two effects combine and result in a temporary slowing, or even extinction, of detonation past the transition region. Depending on the explosive, a region of undetonated explosive may result where the diffraction fails to 'corner turn' and allow prompt reaction. This undetonated region has been termed a dead-zone. At later times, it is highly probable that in any realistically sized explosive system, the dead-zone will combust, but the resulting energy cannot support the lead shock front and may result in a significantly different result downstream than would occur in an explosive that is better at corner turning.

Modeling the corner turning of explosives is complex since the governing equations must be accurate enough both to create a finite reaction zone with correct sound-speeds to allow releases, and to account for the effects of divergence on the local energy release rate. Deficiencies in either of these effects will result in a severely distorted model prediction compared with reality.

The most comprehensive paper on approaches to modeling the detonative behavior of NM is by Menikoff and Shaw [7]. A reactive burn model, such as suggested by Menikoff, is essential if real three-dimensional or overdriven detonative behavior is to be simulated. The computationally faster and easier approach of a programmed burn, often coupled with a simple JWL EOS, has very limited applicability, except at charge sizes so large that detailed physical

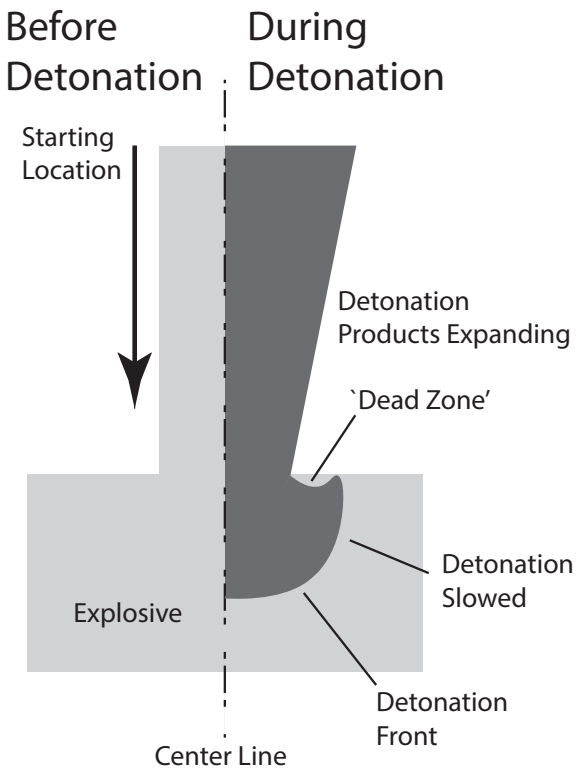

Figure 1: An illustration of the corner turning process in a hypothetical cylindrical geometry. Left: The starting geometry. Right: Detonation has progressed from the top, but has not yet consumed all the explosive.

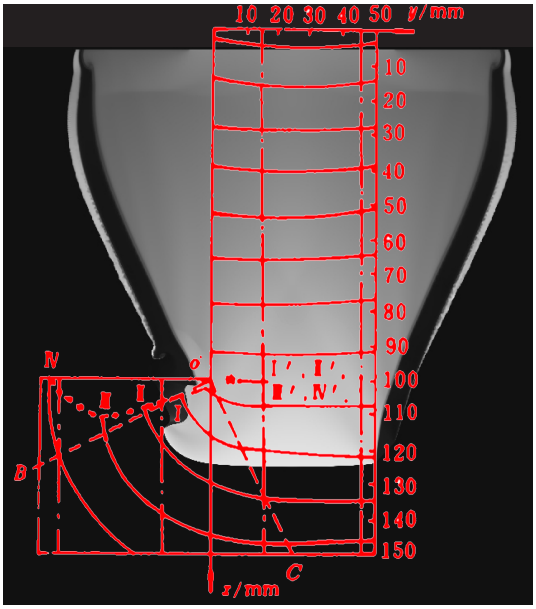

Figure 2: A comparison of the detonation position in an experimental corner turning experiment and the model prediction at 19.25 μs.

phenomena can be ignored.

Recently, the approach of Menikoff was implemented into a general explosive modeling code and used to predict the corner turning behavior noted in [23]. In the experiments, a NM-filled transparent 50 mm cross-section box fed into a 100 $\times$ 50 mm box and the corner turning and the detonation front location were recorded (isochrones) every 2 μs by high-speed photography. The same geometry was modeled and the results compared. Figure 2 shows the comparison at 19.25 μs of model time when the detonation had begun to turn the corner. The model output, in gray-scale, represents temperature, a good prediction of the shock front location likely to be recorded on a high-speed camera since the intensity of light is a strong function of material temperature. Figures 3 and 4 show the results at 21.25 and 23.25 μs respectively. In these examples, a uniform discrepancy between the experimental and model location versus time is not important owing to different time-zero starts; rather, it is how parallel the model detonation shock front and the experimental isochrone is that indicates model predictive accuracy.

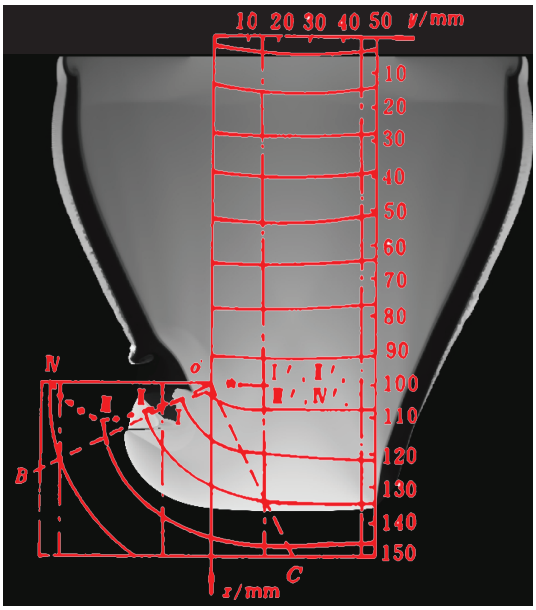

Figure 3: A comparison of the detonation position in an experimental corner turning experiment and the model prediction at 21.25 μs.

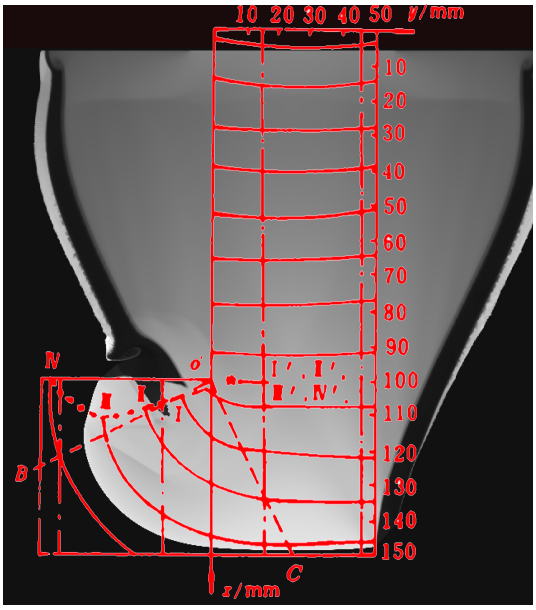

Figure 4: A comparison of the detonation position in an experimental corner turning experiment and the model prediction at 23.25 μs.

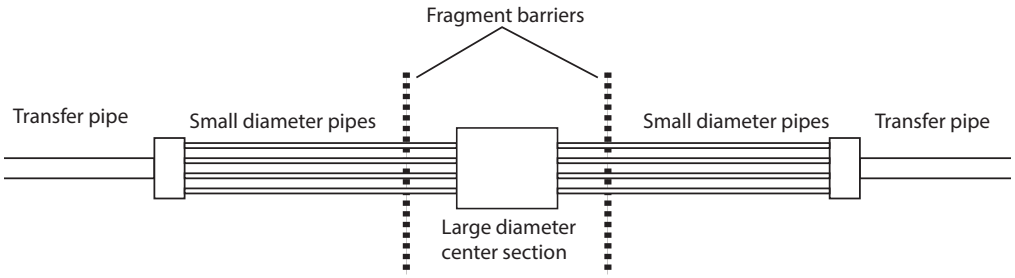

Figure 5: A schematic of the NM detonation trap designed to prevent an accidental detonation at one location transferring to another through a connecting pipe. Liquid being transferred is separated into a number of small diameter pipes, recombined in a central NM filled cavity and then split out again. An accidental detonation at one end is supported in the small pipes, but fails upon entering the central NM cavity owing to the divergent nature of the corner turning process occurring and the substantially different critical diameter for NM in dense walled tubes compared with self-confinement.

It is clear from figure 2 that the model is not slowing the detonation front adequately away from the central axis after turning the corner. That is, the model divergence effect appears to not be severe enough. Oddly, the model appears to over-predict the size of the dead-zone at this time, an apparently opposite fault of quenching the reaction too much. The comparisons in figures 3 and 4 indicate that the overly fast detonation in the off-axis region propagates forward in time and that the shape of the dead-zone is incorrect. In figure 4 detonation appears to have penetrated into a region apparently not seen to detonate in the experiment.

The current model therefore appears to disagree significantly with the experiment. This may just be a sub-optimal choice of fitting parameters and quickly fixed. However, a possibly unrelated but severe non-physical effect is noted as the model mesh resolution is increased to study prediction convergence. This indicates a possible, more fundamental problem with the current implementation. At this time, the development of the model has been ceased owing to budgetary and time constraints. In summary, accurately modeling the corner turning behavior of NM is not trivial.

The corner turning effect is used in the industrial transport of NM between storage locations. The idea is to stop an accidental detonation in one area of the plant being able to transfer within the NM containing pipe to other locations. The device used is called a detonation trap (see figure 5) and comprises a fan-out of numerous small diameter pipes from a larger transport one, and a recombination in a short, wider, NM-filled cylindrical tank (perhaps 250 mm in diameter) before a long further fan-out of smaller pipes to the continuing transport pipe. Numerous small pipes (perhaps 12) are used to allow reasonable flow to occur despite the small cross-section of each (ID 9-12 mm).

As discussed in this document, the critical diameter of NM is very small in cylinders with dense walls (2-3 mm in steel pipes). Therefore an accidental detonation starting at either end of the transport pipe will propagate down the long, small-diameter pipes. However, when the detonation reaches the middle NM-filled cylindrical tank, the detonation will fail to propagate owing to the corner turning process required to break out into the large diameter and the much larger critical diameter of NM when only self-confined (>20 mm). In this way, an accidental detonation from either end of the system is quenched at the center recombination cylinder. The use of barriers and a small diameter pipe length that is sufficient means that fragments created at the exploding pipe end cannot strike the pipes on the other side of the trap with sufficient velocity to induce SDT.

Cellular Detonation

The optical transparency of unreacted NM and transparent confinement, such as PMMA or Pyrex, has led to numerous photographic examinations of the detonation process. An early question related to the effect of diluting the NM explosive with a non-detonable compatible transparent liquid such as acetone [24]. It was discovered that although a macro-scale steady detonation progressed to quite large dilutions, the progress was via microscopic shock wave interactions leading to higher pressures and temperatures that supported

otherwise dying detonations in between [25]. This process has been termed 'cellular detonation' since the pressure patterns left on the walls of the confinement produced a pattern reminiscent of biological cells. Such a phenomenon is commonly observed in gas-phase detonations. The process was explained as a result of initially isolated pockets of detonation from a precursor high pressure shock failing to propagate fully, but the resulting shocks interacted with each other some distance away and increased the temperature enough locally that new isolated detonations were produced. Such isolated triple-point interaction generated detonations and interactions with the boundary conditions resulted in a regular three-dimensional shock front structure being formed quickly. The energy so released allows reaction to occur later in the lower temperature regions between the cell boundaries, and this late time energy helps support the overall macroscopic detonation process, albeit at a lower VOD than for pure NM.

In addition to direct observation of this cellular detonation process, modeling efforts have also supported the experimental observations when suitable boundary and reaction pathway processes are simulated [26]. Since the observed cell size increased with increasing dilution, it was hypothesized that detonation progression, even in undiluted NM, occurred as a result of an increasingly microscopic cellular process [24]. It now appears likely that this hypothesis is incorrect for pure NM in view of the reaction zone data described previously. A cellular detonation front is a three-dimensional event with lateral as well as axial structure. Such a structure, even on a microscopic scale, would be expected to lead to statistical variability in the particle velocity at an window interface such as measured in [22, 18]. In particular, it might lead to a smearing of the leading shock front owing to an imposed phase velocity at the window interface. Since this variability does not occur, it suggests that, at least in pure NM, an essentially flat front to the detonation process occurs.

The shock sensitivity of NM/Methanol mixtures have been measured and found to be similar to those of pure NM [27].

Homogeneous Versus Heterogeneous Detonation

Measuring the temperature created by the application of a shock to materials is difficult. Usually it is even more difficult in explosives because they are by definition capable of exothermic behavior. NM is a rare exception since it is optically transparent, allowing the temperature to be estimated from suitable measurements of the emission of thermal radiation [20, 17]. These types of measurement allow insight into the homogeneous response of NM and validation of predictions based on EOS parameters and Arrhenius kinetic-based ignition criteria.

Reference [17] presents useful insights into the ignition and propagation mechanisms in NM. Shock pressures of between 8.5 & 12 GPa were created in 99% pure NM and monitored with a six wavelength, 3 ns rise-time pyrometer capable of resolving temperatures between 1500 and 6000K. It had been assumed that the process of detonation build-up in homogeneous explosives is as follows [28]. A strong shock enters the homogeneous explosive medium and results in bulk heating. The currently inert shock traverses the explosive at a fixed speed determined by the input shock pressure and the unreacted NM EOS. Provided that the shock is sustained for long enough, the material close to the shock input face has been at elevated temperature for longer than other material and so the exothermic kinetics of reaction begin there first. Detonation results, but occurs in material at a higher than ambient density owing to the unreleased local shock state. This, in turn, produces a super-detonation that proceeds at high velocity to catch the leading strong shock. After overtaking the lead shock, release processes result in the formation of a steady-state detonation that proceeds in the ambient density material.

The pyrometry data show that this description of the formation process is not quite accurate. The temperature measured close to the input face is too high to be created just from bulk heating (EOS-based calculation methods suggest 1000-1100K while 1500-2500K is actually measured). This suggests that some form of energy localization is occurring leading to hot-spots in the NM.

Indeed, when the NM was vacuum degassed, or the input metal face polished to reduce surface roughness that could lead to microscopic shock focusing, the effect was reduced, but not totally eliminated. These treatments did not affect the time to ignition at high input pressures (close to CJ pressures), but did at 9 GPa, suggesting that some enhancement to the marginal ignition kinetics was occurring close to the input shock face from such heterogeneities. The fact that these locally high temperatures did not lead to prompt detonation suggests that they must be sufficiently minute to be sub-critical (i.e. as local hot-spot reaction expands, the thermal losses exceed thermal energy available from reaction). The surface roughness effect is also described in reference [28], and the observation that initial hot-spots observed by pyrometry are likely to be sub-critical is consistent with an observation that gas-filled bubbles of greater than 0.5 mm were required to initiate detonation for an input pressure of approximately 8 GPa. Further, close inspection of the other diagnostics in the pyrometry experiments suggests that super-detonation did not start exactly at the input face where that material was hottest for longest, but in fact some small distance away (0.5-2$\pm$1 mm). The distance appeared to increase for lower pressure input shocks, but the large error bar makes that difficult to prove at this time. This suggests some kind of distributed buildup of reaction energy needs to take place after ignition, but before detonation can occur. This disagrees with the observations of [28] which states that super-detonation occurs directly at the input interface, but agrees with some observations in reference [29].

As described previously, established detonation in NM progresses as a bulk thermally driven process since the irregularities (microscopic bubbles etc.) present in an unperturbed liquid are too small to be practically relevant. However, the addition of solid particles disturbs the regularity and allows the effects of shock wave interactions within the mixture to become significant. It is therefore possible to probe the effects of such particles by varying the concentration, impedance, composition and structure of such additions. This has been done by numerous researchers and it has been shown that the

resulting macroscopic behavior of NM can be changed from a homogeneous to a heterogeneous detonation propagation mechanism [8, 5]. As expected, the addition of such particles sensitizes the NM to the application of shocks and can result in a mixture that is blasting cap sensitive. In reference [5], a transition in detonation behavior (homogeneous to heterogeneous) was observed by the addition of sparse solid beads to the NM as the input shock strength was varied.

References

[1] T. R. Gibbs, A. Popolato, LASL Explosive Property Data, University of California, USA, 1980.

[2] R. R. Ijsselstein, Sensitivity of nitromethane for low velocity detonation, Propellants, Explosives and Pyrotechnics 10 (1985) 14–17.

[3] Angus technical data sheet: Nitromethane, Tech. Rep., ANGUS Chemical Company (2016).

[4] J. Hershkowitz, B. M. Dobratz, Compendium of nitromethane data relevant to the tactical explosive system (TEXS) program, Tech. Rep., ARFSD-SP-89001, AD-B131923 (1989).

[5] D. M. Dattelbaum, A. Sheffield, S, D. B. Stahl, A. M. Dattelbaum, W. Trott, R. Engelke, Influence of hot spot features on the initiation characteristics of heterogeneous nitromethane, in: Forteenth Symposium (International) on Detonation, 2010, Coeur d'Alene, ID, USA, ONR.

[6] A. W. Gibb, An experimental study of corner-turning in nitromethane, PML 1986-44, Tech. Rep., Prins Maurits Laboratorium, TNO, Netherlands (1986).

[7] R. Menikoff, S. M. Shaw, Modeling detonation waves in nitromethane, Combustion And Flame 158 (2011) 2549–2558.

[8] B. W. Asay, D. J. Pauley, E. N. Ferm, Jet initiation thresholds of nitromethane, in: Tenth International Detonation Symposium, 1993, Boston, MA, USA.

[9] J. J. Lee, J. Jiang, K. H. Choong, J. H. S. Lee, Effect of diethylenetriamine and triethylamine sensitization on the critical diameter of nitromethane, AIP Conference Proceedings 505 (1999) 797–800.

[10] R. Engelke, A. Sheffield, S, H. L. Stacy, J. P. Quintana, Reduction of detonating liquid nitromethane's chemical reaction-zone length by chemical sensitization, Physics of Fluids 17 (2016) 096102.

[11] L. Fried, P. Souers, CHEETAH: A next generation thermochemical code, UCRL-ID-117240, LLNL, Tech. Rep. (1994).

[12] R. Engelke, A. Sheffield, S, H. L. Stacy, Effect of deuteration on the diameter-effect curve of liquid nitromethane, J. Phys. Chem. A 110 (2006) 7744–7748.

[13] A. W. Campbell, M. E. Malin, T. E. Holland, Detonation in homogeneous explosives, in: Fifth Symposium (International) on Detonation, 1955, Washington, DC, USA, ONR, pp. 454–477.

[14] A. W. Campbell, M. E. Malin, T. E. Holland, Temperature effects in the liquid explosive, nitromethane, J. App. Phys. 27 (8) (1956) 963–963.

[15] O. E. Petel, A study of the failure mechanism of detonations in homogeneous and heterogenious explosives. Dept. Mech. Eng., McGill University, Quebec, Canada, Ph.D. thesis (2006).

[16] L. G. Hill, J. B. Bdzil, W. C. Davis, R. Engelke, D. L. Frost, Front curvature analysis and detonation shock dynamics calibration for pure and sensitized nitromethane, AIP Conference Proceedings 505 (2000) 813–816.

[17] B. Leal-Crouzet, G. Baudin, Shock initiation of detonation in nitromethane, Combustion And Flame 122 (2000) 463–473.

[18] S. A. Sheffield, R. Engelke, R. R. Alcon, R. L. Gustavsen, D. L. Robins, D. B. Stahl, H. L. Stacy, M. C. Whitehead, Particle velocity measurements of the reaction zone in nitromethane, in: Twelfth International Detonation Symposium, San Diego, CA. USA, 2002.

[19] P. C. Lysne, D. R. Hardesty, Fundamental equation of state of liquid nitromethane to 100 kbar, J. Chem. Phys. 59 (12) (1973) 6512–6523.

[20] J. M. Winey, G. E. Duvall, M. D. Knudson, Y. M. Gupta, Equation of state and temperature measurements for shocked nitromethane, J. Chem. Phys. 113 (2000) 7492–7501.

[21] N. Desbiens, E. Bourasseau, J. Maillet, L. Soulard, Molecular based equation of state for shocked liquid nitromethane, J. Hazardous Mat. 166 (2009) 1120–1126.

[22] V. Bouyer, A. Sheffield, S, D. M. Dattelbaum, R. L. Gustavsen, D. B. Stahl, M. Doucet, L. Decaris, Experimental measurements of the chemical reaction zone of detonating liquid explosives, AIP Conference Proceedings 1195 (2009) 177–180.

[23] Z. Tonghu, Y. Chuan, H. Lishi, S. Chengwei, Experiments and numerical simulations on the diffraction of detonation waves in nitromethane, Explosion and Shock Waves (In Chinese) 14 (2) (1994) 169–174.

[24] W. C. Davis, Fine structure in nitromethane/acetone detonations, in: Seventh Symposium (International) on Detonation, 1981, Annapolis, MA, USA, ONR.

[25] S. N. Buravova, Structure of the detonation wave front in a mixture of nitromethane with acetone, J. of Applied Mechanics and Technical Physics 53 (5) (2012) 633–641.

[26] R. H. Guirguis, Investigation of the thermal initiation of detonation in nitromethane, Tech. Rep., Jaycor, VA, USA. AD-A136211, J206-83-011/6223 (1983).

[27] D. M. Dattelbaum, A. Sheffield, S, B. D. Bartram, L. L. Gibson, P. R. Bowden, B. F. Schilling, The shock sensitivities of nitromethane/methanol mixtures, J. Phys.: Conf. Ser 500 (2014) 182009.

[28] A. W. Campbell, W. C. Davis, J. R. Travis, Shock initiation of detonation in liquid explosives, Physics of Fluids 4 (1961) 498–510.

[29] A. Sheffield, S, R. Engelke, R. R. Alcon, In-situ study of the chemically driven flow fields in initiating homogeneous and heterogeneous nitromethane explosives, in: Ninth Symposium (International) on Detonation, 1989, Portland, OR, USA, ONR.